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14. ABSTRACT

New methods for optimizing band structure in photonic crystals with arbitrary material configurations were developed. The methods make use of large-scale nondifferentiable optimization techniques and rely on efficient finite element solvers for computing band structures. New photonic bandgap structures with large gaps were found.

New finite element methods for computing band structures in two- and three-dimensional photonic crystals were developed. These methods are specifically formulated to handle discontinuous media. A complete convergence analysis was carried out. The methods are made efficient by combining subspace iteration techniques with fast Fourier transform preconditioners.

Analysis of a three-dimensional diffraction grating problem and of natural reflectivity constraints in rapidly oscillating dielectric gratings was carried out, providing improved understanding of diffraction gratings and their properties.

15. SUBJECT TERMS

Micro-optical structures, diffraction, optimal design, modeling.

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Modeling and Optimal Design of Micro-Optical Structures

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1 Objectives

This project developed new techniques for the modeling and optimal design of micro-optical structures, focusing mainly on diffraction gratings and photonic crystals.

The primary objectives of this project were as follows:

- Investigate and develop new optimal design methods based on full PDE diffraction models to produce effective, manufacturable diffractive structures.
- Investigate and develop new computational methods for calculating band structures in photonic crystals.
- Investigate and develop new techniques for the optimal design of photonic bandgap structures and other devices with predetermined spectral behavior.

Each of the main objectives were met.

2 Findings and accomplishments

Diffractive optical structures

An analysis which produces a sharp estimate on the maximum reflectivity of rapidly oscillating diffraction gratings was carried out [1]. This bound is important because it provides a strict upper limit on how much energy can be obtained in reflection from a dielectric grating. It thus characterizes the feasible target parameters for optimal design problems involving such gratings. The constraint is obtained by first carefully analyzing the case of layered media, then appealing to homogenization arguments to obtain asymptotic bounds in the limit as the grating period goes to zero.

A complete analysis of a 3D electromagnetic scattering problem in biperiodic media was carried out [5]. The variational problem formulation obtained may be useful for finite element methods for diffraction gratings and 3D photonic crystal slabs.

An extensive review and expository article describing much of our AFOSR-sponsored work on variational methods for diffractive optics problems can be found in [6].

Computational methods for band structure calculations

An efficient new method for band structure calculations in two-dimensional photonic crystals was developed [7]. The method is based on a finite element approximation coupled with a preconditioned subspace iteration technique. The method is capable of handling E- and H-parallel polarizations in general dielectric orthotropic media with arbitrary material configurations. Use of the preconditioned subspace iteration eigenvalue solver makes the method well-suited for use in large-scale optimization algorithms.

Ideas from the two-dimensional method described above were extended to obtain a new method for band structure calculations in three-dimensional photonic crystals [9]. The method allows arbitrary material configurations in rectangular crystal lattices. The method is based on a mixed finite element discretization using edge elements for the field variables and nodal elements for the divergence constraint. The discretization scheme is novel in that edge and nodal elements are augmented by a phase factor associated with the quasimomentum parameter. This forces the scheme to satisfy a verifiable stability condition. A fast preconditioner is implemented using FFTs on a mixed formulation of a constant coefficient problem. Eigenvalues are again found using a subspace iteration technique. The method appears to be competitive with plane-wave decomposition methods currently in wide use.

A complete convergence analysis of the 3D mixed finite element method described above was carried out [10]. The analysis guarantees convergence of discrete approximations to the correct Bloch eigenvalues and eigenmodes as the mesh size is decreased, even in discontinuous media. This is, as far as we know, the first convergence proof for any method for computing band structures in 3D photonic crystals.

Techniques for optimal design of bandgap structures

An optimal design method for two-dimensional photonic band gap structures in E-parallel polarization was developed and analyzed [3]. The method makes use of nonsmooth optimization techniques, and uses the finite element methods described above. The optimal design method enables the determination of periodic dielectric structures with optimized spectral properties, for example maximization of band gaps, assuming a completely arbitrary material configuration. Numerical experiments produced unexpected novel structures with large band gaps.

The optimal design method for photonic crystals in E-parallel polarization was generalized and extended to handle crystals in H-parallel polarization [8]. The H-parallel case is more difficult due to the decreased regularity of eigenfunctions, and the possibility of anisotropic optima. The method developed, in addition to using ideas from nonsmooth optimization, makes use of a homotopic evolution algorithm. The evolution algorithm allows one to continuously deform an initial structure with given spectral properties into a new structure with much different properties, for example producing band-gap structures from initial periodic structures with no band gap. The method was applied to obtain several new crystal configurations with large band gaps, and with multiple band gaps.

Other findings

A new method for inferring information about underground fluid flows in porous media using controlled-source electromagnetic methods was developed [4]. The method allows one to determine the lateral extent of conductive subsurface plumes in a relatively stable manner, by recovering vertically averaged conductivity profiles. The method is relevant to environmental remediation efforts. This work was based on a previously developed method for quantifying flaws in homogeneous plates via eddy currents.

3 Transitions

Some of the computational techniques for grating structures and photonic crystals developed in this project have been adapted and applied in an industrial setting at Honeywell Technology Center. For example, a finite element method based on our work as described in [6] was applied to analyze MEMS-based grating structures intended for use as tunable near-infrared filters for applications in sensors. The results of this modeling effort are described in [2].

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